Towards Understanding Fatigue Crack Initiation

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TOWARDS UNDERSTANDING FATIGUE CRACK INITIATION: A DISCRETE DISLOCATION DYNAMICS STUDY

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ABSTRACT

The investigation of fatigue crack initiation is important to get a fundamentally better insight in fatigue. It has been established experimentally that dislocations play a vital role in this context. We use discrete dislocation dynamics to build a model for fatigue crack initiation from a surface grain. Dislocations are modeled as line singularities in an elastic medium where they can be nucleated, glide or annihilate. The simulation reveals several features that could give rise to fracture initiation and dislocation structure formation. Three different, potential areas of fracture —surface, grain interior and grain boundary— are found which correspond to those found in experiments. The computational expenses currently limit the number of cycles that can be simulated, and therefore do not allow yet for a comparison with experimental results.

INTRODUCTION

Although it is very well documented that fatigue is the reason for the failure of many structures, and although the initiation of the crack is a necessary condition, it is fair to say that fatigue crack initiation still holds many secrets. Extensive experimental studies have revealed that the initiation periode of fatigue starts with the nucleation and accumulation of dislocations, which might form structures, such as the well-documented ladder-like structure [10]. The ladder-like structure is found inside persistent slip bands, which are very localized and carry most of the plastic deformation in a crystal under continued cyclic deformation.

At the free surface of the crystal, the irreversible motion of dislocations leaves behind intrusions and extrusions. In many cases, also protrusions are visible. These are the result of the massive dislocation motion in persistent slip bands, and can reach heights on the order of micrometers. These protrusions appear to be in many cases the preferential sites for the nucleation of a fatigue crack. Laird [7] suggests that cracks are in fact intrusions, which grow further than others and eventually link up. Basinski and Basinski [1] point out that cracks nucleate most likely in the vicinity of relatively thin protrusions, which are formed later in fatigue life and therefore are less likely to contain deep intrusions.

Other scientists link fatigue crack nucleation to the persistent slip band itself. Based on the vacancy dipole model of Essmann et al. [4], the simulations of Repetto and Ortiz [9] lead to the development of an avalanche of material on the free surface, i.e. an protrusion, and they define the acute angle with the surface as the site of crack nucleation. Brown and Ogin [2] find, based on a dislocation array model, a logarithmic singularity at the intersection of the persistent slip band with the surface, which may lead to fatigue crack initiation.

We present here preliminary results of discrete dislocation dynamics simulations that attempt to shed some more light on the nucleation process of a fatigue crack. In this approach, the movement of discrete dislocations within a elastic matrix is used to understand material properties. The movement is governed by the elastic interactions of the dislocations and the

boundary conditions along with some constitutive laws. The model is similar in spirit to that used by Deshpande et al. [3] for fatigue crack growth, with the exception of a cohesive zone. However, the model in [3] presumed the presence of a crack; our focus here is on the crack initiation step.

MODEL

We consider a semi-infinite, two-dimensional strip where we imagine that a single grain is located at the free surface so that plastic flow takes place inside this grain but not in the surrounding grains, which are supposed to be less favorably oriented, see Figure 1. The rectangular grain has three slip systems at 60° from each other (as a two-dimensional model of an fcc crystal), one being favorably oriented at 45° from the tensile direction. The remote stress, parallel to the free surface, is taken to vary with time in a zig-zag fashion with $\sigma_{\min} = -\sigma_{\max}$.

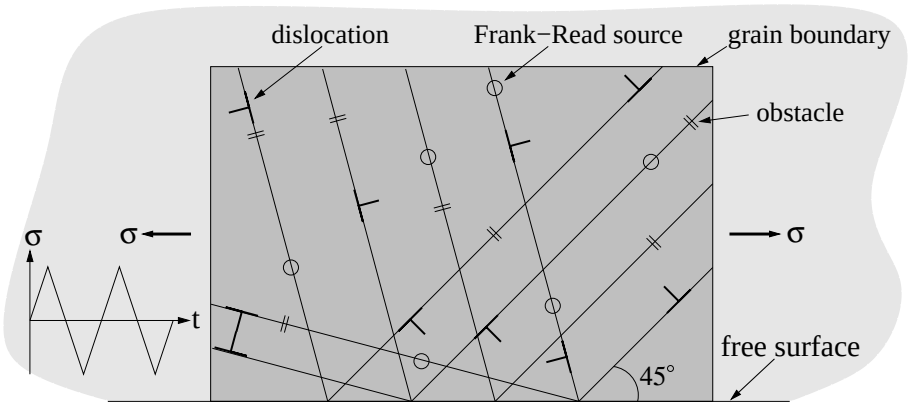

Figure 1: Plane strain strip of material subjected to a remote cyclic tensile stress parallel to the free surface, with a single grain inside of which discrete dislocation dynamics is applied.

Plastic flow inside the grain is caused by the motion of a number of discrete dislocations; the surrounding material remains elastic. All dislocations are of edge character with the Burgers vector in the plane of the model. They are treated as singularities in a linear elastic, plane strain, isotropic continuum. Closed-form expressions are used for the long-range displacement and stress fields in the presence of a traction-free surface [5], so that the boundary conditions are directly taken into account. From these singular stress fields, along with the free surface image stress [6] and the uniform applied stress σ, the Peach-Koehler force on each dislocation is calculated at each instant. This force governs the dislocation motion according to a linear drag relation.

In addition, we incorporate the generation of dislocation dipoles from pre-defined two-dimensional Frank-Read sources, when the resolved shear stress exceeds the source strength τ_{nuc} for a sufficiently long time t_{nuc} (see [11] for details). Dislocations annihilate when the distance between two dislocations of opposite sign is less than a critical distance which is taken to be $6b$. Furthermore, dislocations can escape from the crystal at the free surface, leaving behind a step.

Finally, dislocations can get pinned at point obstacles. These either represent small precipitates or forest dislocations. Grain boundaries are assumed, for simplicity, to be impenetrable by dislocations, thus representing high angle grain boundaries.

The dislocation dynamics is simulated in an incremental fashion using straightforward Euler time integration. The timestep needed is small enough to capture events such as nucleation and junction formation. The dislocation structure that evolves is in no way presumed but is an outcome of the calculation. With the constitutive rules described above, the uniaxial response of the single grain without surrounding material would be close to being elastic-perfectly plastic.

RESULTS AND DISCUSSION

Results are presented for a $2\mu\text{m} \times 2\mu\text{m}$ grain, with the elastic properties being chosen to represent those of aluminum. The grain is dislocation free initially, with dislocation sources (100 per μm^2) and obstacles (75 per μm^2) randomly distributed on a total of 201 slip planes. The source strengths are randomly chosen from a Gaussian distribution and have a mean value of $\tau_{\text{nuc}} = 50\text{MPa}$ and a standard deviation of $0.02\tau_{\text{nuc}}$. All obstacles have a strength of 150MPa. The peak cyclic stress is taken to be $\sigma_{\text{max}} = 150\text{MPa}$.

During the rising branch of the first cycle, the response of the grain is elastic with the resolved shear stresses on the slip planes increasing linearly. When the resolved shear stress reaches the strength of the weakest dislocation source, a dislocation dipole is generated, and one of the two dislocations glides towards the free surface, the other in the opposite direction. Upon further stressing, more dislocations get nucleated and when the first maximal tensile stress is reached roughly 180 dislocations are found inside the grain. During unloading a few dislocations slide back and annihilate. In the compression stage, the dislocation density rises further and subsequently decreases significantly again when unloading from the maximal compressive stress. Nevertheless, after one single cycle there is a net dislocation density. This density accumulates with further cycling, as shown in Figure 2. The accumulated dislocation density increases logarithmically with the number of cycles in the beginning but after around 100 cycles it tails off.

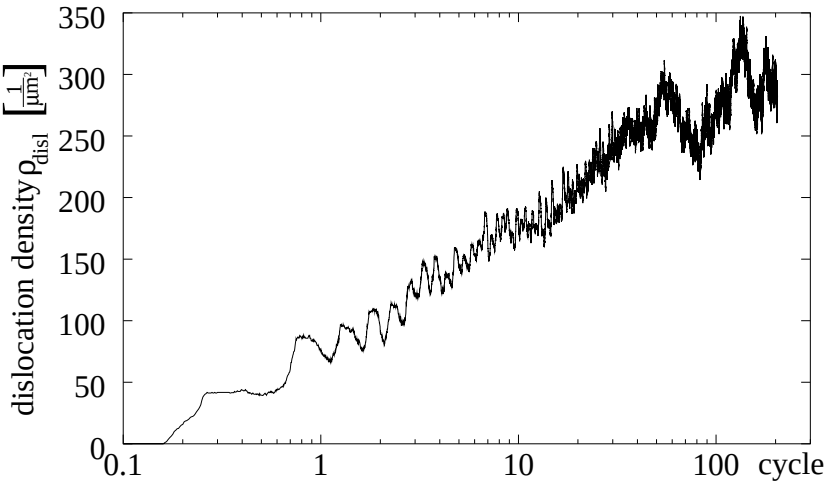

Figure 2: Dislocation density against the number of cycles (logarithmic scale) in the $2\mu\text{m} \times 2\mu\text{m}$ grain.

Fatigue cracks often nucleate inside or near the intersection of the persistent slip band with the surface and follow the primary slip plane. In the model of Fig. 1, this is the one inclined at 45°. To check for the potential nucleation of a crack, we consider the distribution of the

maximal principal tensile stress σ_I. Note that each dislocation carries a $1/r$-singularity, but that a random dislocation distribution gives just a randomly fluctuating stress field that cannot precipitate fracture, since high stresses have to be present over a sufficiently large region. After 325 cycles at zero applied stress, a dislocation distribution has evolved that causes a principal stress field as shown in Figure 3.

In the upper left-hand region of the grain the field is just randomly fluctuating, but there are extensive regions of relatively high tensile stresses near certain parts of the free surface and at the grain boundary. Furthermore, the traces of high-stressed regions inside the grain follow the primary slip system direction. The corresponding principal orientations, which are not shown, are perpendicular to the 45° slip plane. At any rate, the stresses are in the order of the maximal applied stress, but this is too small to cause breaking of inter-atomic bonds.

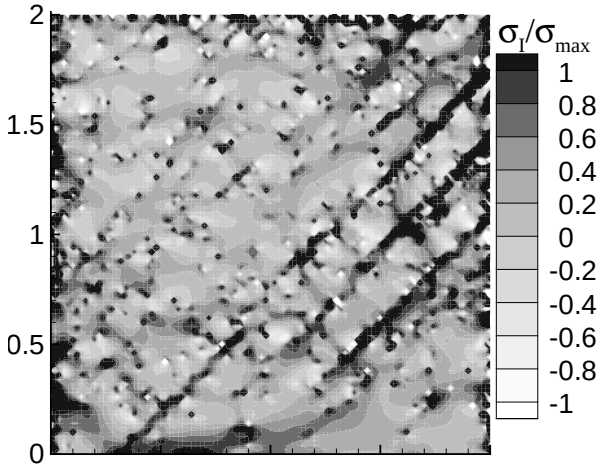

Figure 3: First principal stress σ_I normalized by the maximum applied stress in the grain after 325 cycles. The free surface is on the bottom side.

Since different dislocation structures, such as channel-vein, ladder-like or cell structures [10] are found in fatigued materials, an important goal for this study is to observe if and how such structures develop. As a diagnostic tool, we use the lattice rotation field, which can be directly computed from the superposition of the displacement fields of all dislocations. The idea is that if dislocations are truly randomly distributed, lattice rotation is a random field; on the other hand, if dislocations organize in structures in certain regions, this will become apparent as a region of net rotation. In addition, lattice rotations could also be compared to experiments. The lattice rotation after 325 cycles is shown in Figure 4. The part that is more than 1.5μm from the free surface shows a constant positive rotation while negative rotations prevail at the lower right-hand corner. Overall, there appears to be a majority of positive rotations at this early time in fatigue life.

CONCLUDING REMARKS

The preliminary results reveal the evolution of dislocation structures, which lead to the accumulation of stresses in the grain and at the grain boundary. The stresses are too low for fracture and the structures are not pronounced enough compared to experiments [8]. This can be attributed to the fact that only a relatively small number of cycles has been simulated.

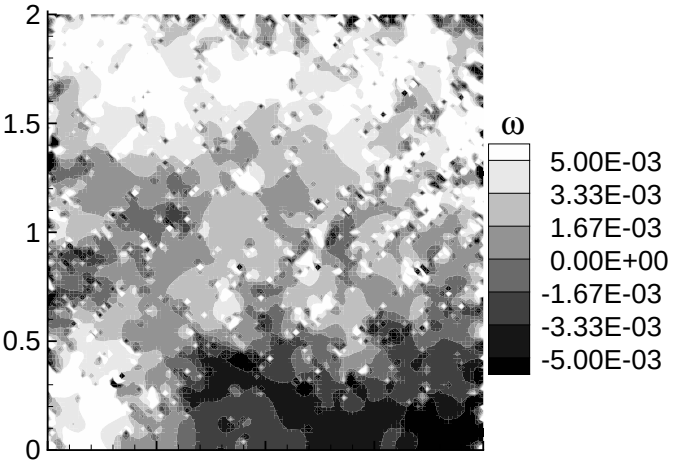

Figure 4: Lattice rotation ω in the grain after 325 cycles. The free surface is on the bottom side.

The model also shows that two distinct fracture mechanisms can occur. As in low-cycle fatigue were mostly transgranular fracture is observed, high stresses are found along traces of the primary slip plane. In high-cycle fatigue, grain boundaries act as sources for fracture leading to intergranular fracture.

Furthermore, the dislocation density increases logarithmically first and gradually seems to saturate, suggesting that large numbers of dislocations are found in fatigued material. The densities calculated here are about a quarter to half of the densities found in experiments. A further increase of dislocation density may occur in later cycles.

This model is computationally very expensive, since all dislocation interactions have to be calculated. This leads to the need of accelerating methods. Besides methods that do not alter the model, like the use of parallel code, other methods are needed which average in time or space (Fast Multipole Method) to achieve shorter calculation times. These averaging procedures have to fulfill the condition that dislocation interaction is still accurately accounted for.

To model fracture, cohesive surfaces have to be included into the model. This in turn requires a finite element method, which corrects for the boundary conditions of the crack [11, 3], but on the other hand further increases the computational expenses.

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